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Screening effect of an electron in the atom

S N Soni[(a,b)] and Y R Al-Abanie[(a)]
[(a)]Department of Physics, Faculty of Science, Garyounis University, P.O.Box No. 9480, Benghazi, Libya
[(b)]Department of Physics, J N Vyas University, Jodhpur-342 003, Rajasthan, India

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Abstract : The contribution to the screening constant σ_1 for a particular X-ray energy level by an individual electron of the same subshell, in which the atom is ionised, has been calculated The results on subshells of L, M, N and O orbits and their systematics have been presented.

Keyword : Screening by electron

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The Sommerfeld screening constants σ_1 and σ_2 for various X-ray energy levels were recalculated in recent past [1,2]. These authors had used the closed formula

$$\frac{(Z-\sigma_1)^2}{n^2} = \frac{E}{\text{Rhc}} + \frac{(Z-\sigma_2)^2}{n^2}$$

$$-\frac{2}{\alpha^2}\left[1-\left\{1+\frac{\alpha^2(Z-\sigma_2)^2}{\left\{n-\left(j+\frac{1}{2}\right)+\left[\left(j+\frac{1}{2}\right)^2-\alpha^2\left(Z-\sigma_2\right)^2\right]^{1/2}\right\}^2}\right\}^{-1/2}\right] \quad (1)$$

In this formula, E represents the energy of a Z-atom having a hole in n, l, j subshell. Other symbols have their usual meaning. Due to this closed formula, the truncation errors, arising out of series expansion formula and present in the earlier results [3] were avoided. While the constant σ_2 has been established in the literature, to represent the screening due to the electrons inner to the hole position, in question, σ_1 represents that due to all the electrons present in the atom. A survey of the values of σ_l [1,2] for a particular X-ray energy level shows that each addition of an electron in a comparatively outer subshell increases σ_l by a constant value. This constancy is more clearly exhibited when electrons are added in subshells much outer to the hole position. Also, this constant value, denoted presently by $\delta\sigma_l$ and presented in Table 1, decreases as the electrons are added to more and more outer

Table 1. Values of $\delta\sigma_l$ for various subshells contributed by an electron in comparatively outer subshells

S.No	Outer subshell in which electron is added	The subshell in which single hole exists :				
		$2s$	$2p$	$3s$	$3p$	$3d$
1	$3d$	0.29	0.30	–	–	–
2	$4s$	0 20	0.20	–	–	–
3	$4p$	0 19	0.20	–	–	–
4	$4d$	0 18	0 18	0 35	0.35	0 35
5	$4f$	0 17	0.17	0.38	0.38	0 38
6	$5s$	0.17	0 17	–	–	–
7	$5p$	0 13	0 14	0.24	0 24	0 20
8	$5d$	0 15	0 15	0 29	0 29	0 29
9	$6s$	0 13	0 13	0 22	-	0 18
10.	$6p$	0 13	0 13	0 27	0 26	0 22

subshells. In the present study, an attempt has been made to estimate the contribution to σ_l for a X-ray energy level by an individual electron orbiting in the same subshell in which the hole exists.

If we consider a triplet state of an atom doubly ionised in any one subshell, it can be assumed that the energy of such an excited atom is equally shared by both the holes present in the subshell. Representing the energy of each hole by the formula (1), the new value of σ_l can be calculated. This value, presently denoted by σ_l', represents the screening of nuclear charge by all the electrons in the atom having two holes in a subshell. The difference $\sigma_l - \sigma_l'$ is taken to represent the screening by that particular electron which was present in the singly ionised atom, in case of σ_l, and is absent in doubly ionised atom, *i.e.* in case of σ_l'.

The energy $E(YY)$ of an atom doubly ionised in Y subshell has been calculated by

$$E(YY) = E(X) - E(X - YY), \qquad (2)$$

where $E(X)$ is the energy of an atom singly ionised in X subshell, and $E(X - YY)$ denotes the $X - YY$ Auger transition energy. These two values have been taken from the Tables of Bearden and Burr [4] and of Larkins [5] respectively. Out of various levels of a YY state, the energy of a ^3L_J level with the highest values of L and J has been taken as $E(YY)$, as this is the most probable state. This value of $E(YY)$ has been halved and used as the energy of each hole in the atom. The value of σ_1', namely the new value of σ_1, has been calculated by formula (1). Finally, the difference $\Delta\sigma_1 = \sigma_1 - \sigma_1'$ has been determined by taking σ_1 from the reports of Gokhale and Misra [1,2]. The calculations have been performed for subshells of L, M, N and O orbits of all those elements for which Auger data [5] are available. In these calculations, values of σ_2 have been taken to be same as those presented by Gokhale and Misra [2] for singly ionised atoms, because σ_2 is independent of Z value of the atom for a particular hole state.

The values of $\Delta\sigma_1$ for various subshells are presented in Figures 1 to 3. It is seen that for $2s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$ subshells, $\Delta\sigma_1$ lies between 0.20 and 0.28. For each of these subshells, the $\Delta\sigma_1$ is higher for lower Z and decreases very slowly with increasing Z. Similar values for M subshells lie in a wider range. The values for low Z are as high as 0.39

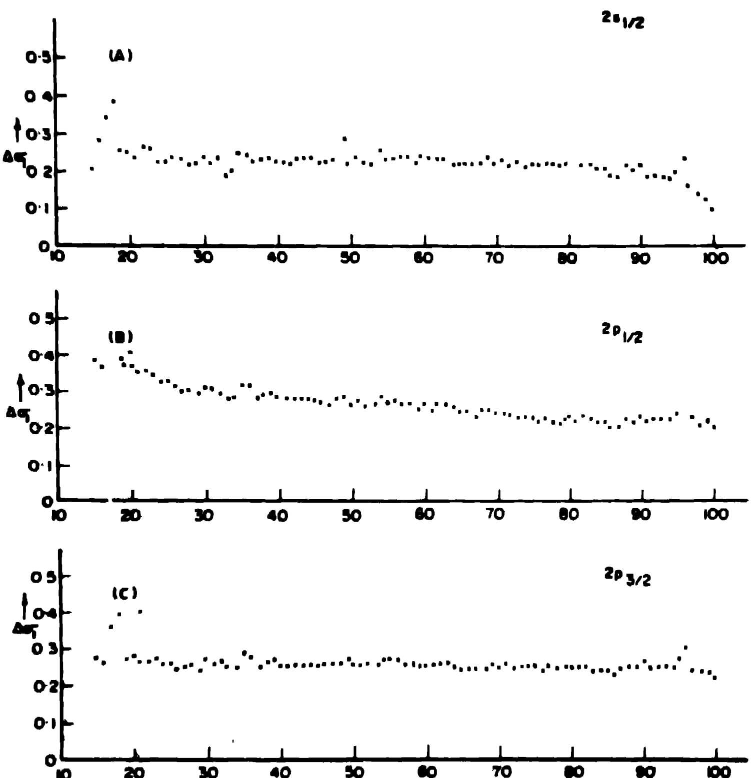

Figure 1. The values of $\Delta\sigma_1$ for an electron in $2s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$ subshells.

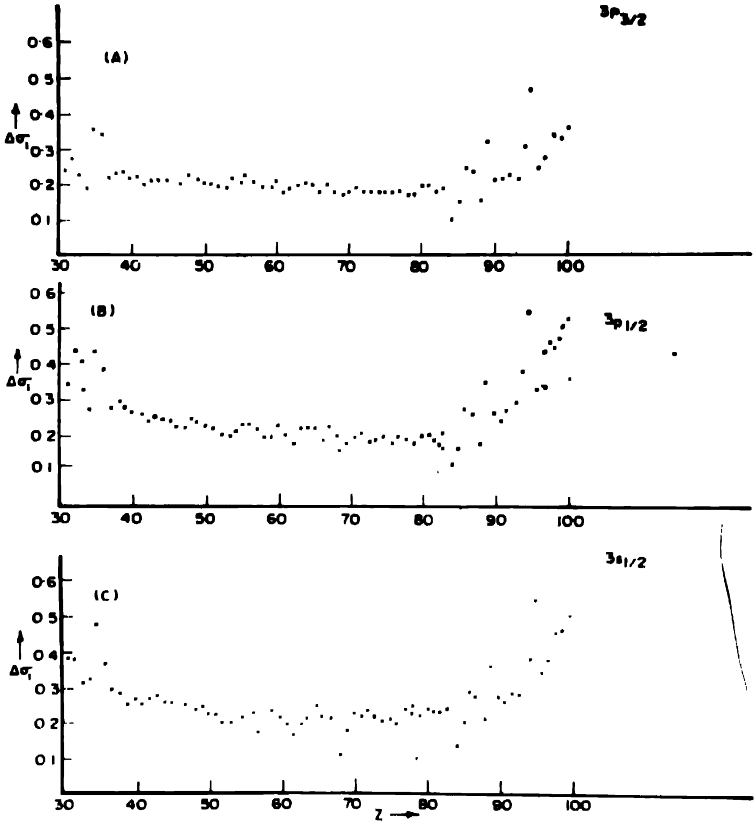

Figure 2. The values of $\Delta\sigma_1$ for an electron in $3s_{1/2}$, $3p_{1/2}$ and $3p_{3/2}$ subshells.

to 0.16 for high Z. These ranges of $\Delta\sigma_1$ for various subshells are presented in Table 2. This behaviour of $\Delta\sigma_1$ is classically understood by the fact that for a higher number of electrons present in the atom, the addition of another electron is less effective in changing the electric

Table 2. Range of $\Delta\sigma_1$ for various subshells in variour elements

S.No	Subshell	No. of elements in which $\Delta\sigma_1$ has been calculated	Range of $\Delta\sigma_1$	
			Minimum	Maximum
1.	$2s_{1/2}$	86	0.20	0.25
2.	$2p_{1/2}$	86	0.20	0.28
3.	$2p_{3/2}$	86	0.22	0.27
4.	$3s_{1/2}$	68	0.21	0.29
5.	$3p_{1/2}$	70	0.17	0.27
6.	$3p_{3/2}$	69	0.16	0.24
7	$3d_{3/2}$	64	0.19	0.39

Table 2. *(Cont'd.)*

S.No.*	Subshell	No. of elements in which $\Delta\sigma_l$ has been calculated	Range of $\Delta\sigma_l$ Minimum	Maximum
8.	$3d_{5/2}$	64	0.20	0.34
9.	$4s_{1/2}$	42	0.00	0.65
10.	$4p_{1/2}$	41	0.17	1.11
11.	$4p_{3/2}$	44	0.08	0.86
12.	$4d_{3/2}$	25	0.10	0.53
13.	$4d_{5/2}$	24	0.14	0.64
14.	$4f_{5/2}$	7	0.49	0.76
15.	$4f_{7/2}$	6	0.00	0.28
16.	$5p_{1/2}$	6	0.66	1.75
17.	$5p_{3/2}$	14	0.04	1.32

*In the results from S.Nos. 1 to 8, while finding the minimum and maximum values of $\Delta\sigma_l$, the values falling outside the systematic behaviour have been ignored.

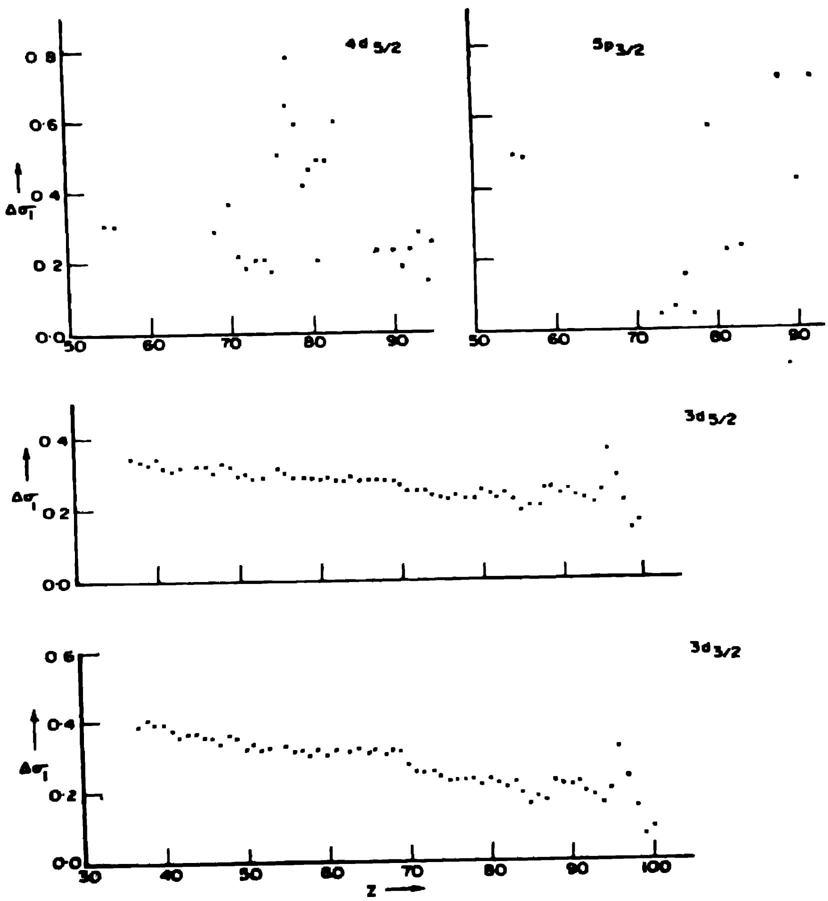

Figure 3. The values of $\Delta\sigma_l$ for an electron in $3d_{3/2}$, $3d_{5/2}$, $4p_{3/2}$ and $5p_{3/2}$ subshells.

changing the electric field. Another feature of the variation of $\Delta\sigma_1$ with Z in these subshells is the oscillating behaviour, as number of electrons increases in a subshell. This oscillating behaviour for a subshell is more pronounced for low Z atoms and the curve begins to smoothen at higher Z values, particularly for those values of Z for which the subshell, in question, lies much deeper.

A very peculiar feature is observed for $j = 1/2$ subshells of M shell. For these subshells, $\Delta\sigma_1$ shows a sharp rise in the range $Z > 85$. In case of $3p_{3/2}$ level, this rise is not so pronounced while $3d_{3/2}$ and $3d_{5/2}$ levels donot show this behaviour. No attempt has been made to explain this behaviour. However, it can tentatively be associated with the ellipticity of the subshells.

Coming to N and O shells, it is observed that $\Delta\sigma_1$ for these subshells vary from as low as 0.00 to as high as ones greater than 1. The data available are in fewer number of elements and $\Delta\sigma_1$ show a very irregular variation with increasing Z. As examples, results for $4p_{3/2}$ and $5p_{3/2}$ subshells are presented in Figure 3. The results for other N and O subshells not presented here, show much larger variations. One reason for this large variation in $\Delta\sigma_1$ may be the error inherent in taking the energy of a two hole state with the highest values of L and J as the energy E in formula (1). The separations of various $^{(2s+1)}L_J$ sublevels relative to their absolute values is more in case of outer orbits and produce larger deviations from average energy. Also the wider range in outer subshells might be due to interpenetrating subshells of atoms which are more overlapping ones in case of N and O subshells. A study of the behaviour of $\Delta\sigma_1$ with increase in Z value can help in understanding this overlapping of the subshells.

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